

# Ground-State Energy and Green's Function for Reduced Hamiltonian for Superconductivity\*

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In their theory of superconductivity, Bardeen, Cooper, and Schrieffer made use of a reduced Hamiltonian which included only scattering of pairs of particles of opposite momentum and spin. It is shown that the solution they obtained by a variational method is correct to  $O(1/n)$  for a large system. The single particle Green's function is derived and used to calculate the interaction energy.

IN their theory of superconductivity, Cooper, Schrieffer, and one of the authors<sup>1</sup> made use of a reduced Hamiltonian which included only scattering of pairs of particles of opposite momentum and spin. They suggested that the solution obtained by a variational method might well be correct to  $O(1/n)$  in the number of particles,  $n$ . They showed in particular that  $\langle H_{\text{red}}^p \rangle$  differs from  $\langle H_{\text{red}} \rangle^p$  by  $O(1/n)$  for  $p=2,3$  and very likely for  $p \ll n$ , where the averages are taken with respect to the variational wave function for the ground state. If this were true for all  $p$ , the energy would be exact. Anderson<sup>2</sup> showed that the reduced problem is analogous to one of a system of interacting spins and gave a physical argument, based on the correspondence principle, which also indicated that the solution is correct to  $O(1/n)$ . Particularly because the validity of the solution has been questioned, we thought it desirable to give a direct proof based on the structure of the wave functions. We also derive the single particle Green's function for the system and use it to calculate the energy of  $H_{\text{red}}$  from an expression given by Galitskii and Migdal.<sup>3</sup>

The reduced Hamiltonian may be written in the form:

$$H_{\text{red}} = \sum_{\mathbf{k}, \sigma} (\epsilon_{\mathbf{k}} + \mu) c_{\mathbf{k}\sigma}^* c_{\mathbf{k}\sigma} + \sum V_{\mathbf{k}\mathbf{k}'} b_{\mathbf{k}\mathbf{k}'}^* b_{\mathbf{k}\mathbf{k}'}, \quad (1)$$

where  $c_{\mathbf{k}\sigma}^*$  is a creation operator for a particle in a state of wave vector  $\mathbf{k}$  and spin  $\sigma$ ,  $b_{\mathbf{k}\mathbf{k}'} = c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$  destroys the pair  $\mathbf{k} \equiv (\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$  and  $\epsilon_{\mathbf{k}}$  is the Bloch energy measured from the Fermi energy,  $\mu$ . For simplicity we assume that the interaction  $V_{\mathbf{k}\mathbf{k}'} = V_{\mathbf{k}'\mathbf{k}}$  is real. The ground-state wave function  $\Psi_0$  of  $H_{\text{red}}$  is a linear combination of configurations in which the single particle states are occupied in pairs of opposite momentum and spin.

Following BCS it is convenient to decompose  $\Psi_0$  into

parts with definite occupancy of a particular pair,  $\mathbf{k}$ :

$$\Psi_0 = u_{\mathbf{k}} b_{\mathbf{k}}^* \varphi_{0\mathbf{k}}(n-2) + v_{\mathbf{k}} \varphi_{0\mathbf{k}}(n), \quad (2)$$

where  $u_{\mathbf{k}}^2 = 1 - v_{\mathbf{k}}^2 = h(\mathbf{k})$  is the probability of occupancy of  $\mathbf{k}$ . Here  $\varphi_{0\mathbf{k}}(n)$  is a function of  $n$  particles in which the pair  $\mathbf{k}$  is not occupied.

The functions  $\varphi_{0\mathbf{k}}$  may be further decomposed into parts with definite occupancy of some other pair  $\mathbf{k}'$ :

$$\varphi_{0\mathbf{k}}(n) = u_{\mathbf{k}\mathbf{k}'} b_{\mathbf{k}\mathbf{k}'}^* \varphi_{0\mathbf{k}\mathbf{k}'}(n-2) + v_{\mathbf{k}\mathbf{k}'} \varphi_{0\mathbf{k}\mathbf{k}'}(n). \quad (3)$$

This function is similar to  $\Psi_0$  except that it contains no configurations in which the pair  $\mathbf{k}$  is occupied. To terms of  $O(1/n)$ , the coefficients of this second decomposition must be independent of  $\mathbf{k}$  and the same as those in (2), i.e.,

$$u_{\mathbf{k}\mathbf{k}'} = u_{\mathbf{k}'} + O(1/n), \quad (4a)$$

$$v_{\mathbf{k}\mathbf{k}'} = v_{\mathbf{k}'} + O(1/n). \quad (4b)$$

This is true because the occupancy of  $\mathbf{k}'$  depends on the interaction of pairs in  $\mathbf{k}'$  with all other pairs, and can be changed only to  $O(1/n)$  if configurations with one pair state, e.g.,  $\mathbf{k}$ , are omitted. In the BCS solution, there is no correlation between the coefficients of the first and second decomposition, which corresponds to omitting the terms of  $O(1/n)$  in (4). The interaction energy to this order is:

$$U = \sum \langle 0 | V_{\mathbf{k}\mathbf{k}'} b_{\mathbf{k}\mathbf{k}'}^* b_{\mathbf{k}\mathbf{k}'} | 0 \rangle = \sum V_{\mathbf{k}\mathbf{k}'} [u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'} + O(1/n)]. \quad (5)$$

As the size of the system is increased, keeping the particle density constant, the matrix element  $V_{\mathbf{k}\mathbf{k}'}$  is inversely proportional to volume and thus to  $n$ , so that the total interaction energy is proportional to  $n$ . The terms of  $O(1/n)$  would contribute only a constant energy, independent of volume.<sup>4</sup>

To calculate the Green's function,<sup>5</sup> we need the

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<sup>1</sup> J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957). We refer to this paper as BCS.

<sup>2</sup> P. W. Anderson, Phys. Rev. **110**, 827 (1958).

<sup>3</sup> V. M. Galitskii and A. B. Migdal, J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 139 (1958) [translation: Soviet Phys.—JETP **34**(7), 96 (1958)]. V. M. Galitskii, J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 145 (1958) [translation: Soviet Phys.—JETP **7**, 104 (1958)].

<sup>4</sup> It should be noted that a similar argument cannot be applied to the complete Hamiltonian. There are then  $n^2$  interaction terms and errors of  $O(1/n)$  can pile up to give a correction proportional to  $n$ . In fact, almost the entire normal-superconducting transition energy comes from the interaction terms in  $H_{\text{red}}$ , and these contain only  $O(1/n)$  of the total interaction.

<sup>5</sup> The Green's function for  $H_{\text{red}}$  has been derived by others, e.g., L. P. Gorkov, J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 735 (1958) [translation: Soviet Phys.—JETP **34**(7), 505 (1958)], by use of wave functions with variable numbers of particles. It is believed that the present derivation is new.

matrix elements of  $c_{k\sigma}^*$  and  $c_{k\sigma}$  which connect the ground-state  $\Psi_0$  of  $n$  particles with excited states of  $n+1$  and  $n-1$  particles, respectively. The excited states of interest are what are called single particle excitations in BCS and consist of linear combinations in which one state of a given pair is occupied in all configurations and the other is not. Thus, we shall denote by  $\Psi(\mathbf{k}\sigma, n+1)$  an excited state of a system of  $n+1$  particles in which  $\mathbf{k}\sigma$  is certainly occupied and the remaining particles are in ground pair configurations. It should be noted that there are no terms in  $H_{\text{red}}$  which scatter an electron in a singly occupied state. It is this fact which makes possible the determination of the excitation energies and matrix elements to  $O(1/n)$  from the structure of the wave functions without use of a perturbation or diagram expansion.

We shall use Lehmann's expression for the momentum-energy representation of the single-particle Green's function in a form given by Galitskii<sup>3</sup>:

$$G(k, \epsilon) = \int_0^\infty dE \left( \frac{\rho^+(\mathbf{k}, E)}{E - \epsilon - i\delta} - \frac{\rho^-(\mathbf{k}, E)}{E + \epsilon - i\delta} \right), \quad (6)$$

where  $\rho^+(\mathbf{k}, E)$  and  $\rho^-(\mathbf{k}, E)$  are defined by

$$\rho^+(\mathbf{k}, E) dE = \sum_{\mathbf{k}} |(\mathbf{k}, n+1 | c_{\mathbf{k}}^* | 0)|^2, \quad E < E_{\mathbf{k}} < E + dE; \quad (7a)$$

$$\rho^-(\mathbf{k}, E) dE = \sum_{\mathbf{k}} |(\mathbf{k}, n-1 | c_{\mathbf{k}} | 0)|^2, \quad E < E_{\mathbf{k}} < E + dE. \quad (7b)$$

The single particle energies,  $E_{\mathbf{k}}$  are defined by<sup>6</sup>

$$E_{\mathbf{k}} = W(\mathbf{k}, n+1) - W_0(n) - \mu, \quad (8a)$$

$$E_{\mathbf{k}} = W(\mathbf{k}, n-1) - W_0(n) + \mu, \quad (8b)$$

in which  $W(\mathbf{k}, n\pm 1)$  are energies of  $\Psi(\mathbf{k}, n\pm 1)$  and  $W_0$  is the ground-state energy of  $H_{\text{red}}$ .

To terms of  $O(1/n)$ ,

$$\begin{aligned} \Psi(\mathbf{k}\uparrow, n+1) &= c_{\mathbf{k}\uparrow}^* \varphi_{0\mathbf{k}}(n), \\ \Psi(\mathbf{k}\uparrow, n-1) &= c_{-\mathbf{k}\downarrow} \varphi_{0\mathbf{k}}(n), \end{aligned} \quad (9)$$

so that the matrix elements are

$$(\mathbf{k}\uparrow, n+1 | c_{\mathbf{k}\uparrow}^* | 0) = u_{\mathbf{k}} = [1 - h(\mathbf{k})]^{\frac{1}{2}}, \quad (10a)$$

$$(\mathbf{k}\uparrow, n-1 | c_{-\mathbf{k}\uparrow} | 0) = v_{\mathbf{k}} = h(\mathbf{k})^{\frac{1}{2}}. \quad (10b)$$

Thus

$$G(\mathbf{k}, \epsilon) = \frac{1 - h(\mathbf{k})}{E_{\mathbf{k}} - \epsilon - i\delta} - \frac{h(\mathbf{k})}{E_{\mathbf{k}} + \epsilon - i\delta}. \quad (11)$$

The energies  $W_0(n)$  and  $W(\mathbf{k}, n+1)$  may be expressed

<sup>6</sup> Our  $E_{\mathbf{k}}$  is identical with  $E_s$  of Galitskii (reference 3).

in the form:

$$W_0(n) = W_{0\mathbf{k}}(n) + 2\epsilon_{\mathbf{k}}h(\mathbf{k}) + U_{\mathbf{k}}, \quad (12)$$

$$W(\mathbf{k}, n+1) = W_{0\mathbf{k}}(n) + \epsilon_{\mathbf{k}} + \mu. \quad (13)$$

Here  $W_{0\mathbf{k}}(n)$  is the energy corresponding to  $\varphi_{0\mathbf{k}}(n)$  and is what the ground-state energy of the system would be if the state  $\mathbf{k}$  were omitted from the Hamiltonian. The last two terms of (12) represent the contributions of the kinetic energy and of the interaction energy  $U_{\mathbf{k}}$  from the pair state  $\mathbf{k}$  to  $W_0$ . The expression (13) follows because the singly occupied state  $\mathbf{k}$  cannot contribute to the pair interaction energy of  $H_{\text{red}}$  and the Fermi energy  $\mu$  is unchanged to  $O(1/n)$  if one particle or one state is added or subtracted from the system. From (8) we find

$$E_{\mathbf{k}} - \epsilon_{\mathbf{k}} = -2\epsilon_{\mathbf{k}}h(\mathbf{k}) - U_{\mathbf{k}}. \quad (14)$$

The explicit expression for  $U_{\mathbf{k}}$  is

$$\begin{aligned} U_{\mathbf{k}} &= (0 | \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} b_{\mathbf{k}'}^* b_{\mathbf{k}'} + \sum_{\mathbf{k}'} V_{\mathbf{k}'\mathbf{k}} b_{\mathbf{k}'}^* b_{\mathbf{k}'} | 0) \\ &= 2 \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} [h(1-h)h'(1-h')]^{\frac{1}{2}} + O(1/n). \end{aligned} \quad (15)$$

Another expression for  $U_{\mathbf{k}}$  can be obtained from the equations of motion for  $G$ , or, perhaps more directly, for  $c_{\mathbf{k}}$ . For a pair interaction,

$$\begin{aligned} U_{\mathbf{k}} &= [0 | (H, c_{\mathbf{k}}^*) c_{\mathbf{k}} - c_{\mathbf{k}}^* (H, c_{\mathbf{k}}) - 2(\epsilon_{\mathbf{k}} + \mu) c_{\mathbf{k}}^* c_{\mathbf{k}} | 0] \\ &= [0 | H c_{\mathbf{k}}^* c_{\mathbf{k}} - 2 c_{\mathbf{k}}^* H c_{\mathbf{k}} + c_{\mathbf{k}}^* c_{\mathbf{k}} H \\ &\quad - 2(\epsilon_{\mathbf{k}} + \mu) c_{\mathbf{k}}^* c_{\mathbf{k}} | 0]. \end{aligned} \quad (16)$$

For our case, this reduces to

$$\begin{aligned} U_{\mathbf{k}} &= h(\mathbf{k}) [2W_0 - 2(E_{\mathbf{k}} - \mu + W_0) - 2(\epsilon_{\mathbf{k}} + \mu)] \\ &= -2(\epsilon_{\mathbf{k}} + E_{\mathbf{k}})h(\mathbf{k}). \end{aligned} \quad (17)$$

The same result may be obtained by an expression derived by Galitskii and Migdal<sup>8</sup> for pair interactions in terms of the Green's function:

$$U_{\mathbf{k}} = \frac{i}{2\pi} \int_C (\epsilon - \epsilon_{\mathbf{k}}) G(\mathbf{k}, \epsilon) d\epsilon. \quad (18)$$

The integral is over a contour  $C$  in the complex  $\epsilon$  plane which consists of the real axis and a semicircle over the upper half-plane.

By combining (14) and (17), we get the same relation between  $E_{\mathbf{k}}$  and  $h(\mathbf{k})$  that was found by BCS from their variational method:

$$h(\mathbf{k}) = \frac{1}{2} [1 - (\epsilon_{\mathbf{k}}/E_{\mathbf{k}})]. \quad (19)$$

Finally, from (14), (15), and (17), we obtain an integral equation for  $h(\mathbf{k})$  which is the same as Eq. (2.33) of BCS.

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